Comparisons of Augmented Pairs Designs and Subset Designs

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Abstract

A response surface design from one of the classes available in the literature can be a natural choice for many experimenters. Augmented Pairs designs were constructed for modeling second order response surfaces and shown to have several desirable properties. Here, Augmented Pairs designs for 3-6 factors are compared with designs of the same size selected from the class of Subset Designs. Designs are compared on the basis of different information based optimality criteria and graphical criteria in spherical and cuboidal regions. Many useful subset designs of the same size are better than the AP design. The user can think of a variety of properties to make a better choice of designs of a particular size from among these two classes.
Keywords: Augmented pairs design; Subset design; Information based optimality; Variance dispersion graph; Fraction of design space plot.

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1. Introduction

Many experiments in the chemical industry, food science, medicine, life sciences, etc. involve a relatively small number of factors, especially when a response surface is to be explored. The users of designed experiments are faced with a common problem of choosing a suitable design from among many of the same size. A design which performs well under some desirable optimality criteria may be a natural choice, but simply choosing an optimal design might not give enough consideration to the range of good properties the design should have. Many information based

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criteria and graphical methods are used for comparing response surface designs. Graphical comparison of response surface designs has become quite popular since **the work of** Giovannitti-Jensen and Myers (1989), **they** mentioned that variance dispersion graphs can provide more information about a design than scalar optimalities. Khuri et al. (1996) constructed quantile dispersion graphs to describe the distribution of prediction variance at different radii from the design center. Zahran et al. (2003b) introduced fraction of design space plots which show fraction of design space at or below each prediction variance value.

This study presents a comparison of the Augmented Pairs (AP) designs of Morris (2000) for three and four factors with designs selected of the same size from a rich class of designs called Subset Designs proposed by Gilmour (2006). Many subset designs are considered, which are of the same size as AP designs, so that the user can have a better choice with the same economic constraints with regard to design size. The two classes of designs are compared on the basis of many numeric as well as graphical comparisons in spherical and cuboidal regions of experimentation. Section 2 of the paper presents the model structure of AP designs and subset designs. Section 3 describes the different optimality criteria to be used for comparison. Sections 4 provides some examples, for spherical and cuboidal regions respectively, showing the comparison of the classes of designs for specific values of k. In Section 5, a brief discussion concerning the choice of design from among these two classes and some concluding remarks are presented. Subset designs of several sizes have been compared under variety of optimality criteria in the Appendix B. Appendix B is presented on website: `https://figshare.com/account/home#/data`.

2. Second-Order Response Surface Designs

Second-order response surface designs are a popular choice among the practitioners to estimate the second-order polynomial model. The second-order polynomial for expected response y is

$$E(y|\mathbf{x}) = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum_{i=1}^{k-1} \sum_{j=i+1}^{k} \beta_{ij} x_i x_j.$$

In matrix notation

$$E(\mathbf{y}|\mathbf{X}) = \mathbf{X}\boldsymbol{\beta},$$

where $\boldsymbol{\beta}$ is the vector of p=$(k+2)(k+1)/2$ regression coefficients of order $p\times 1$, we may write as

$$\boldsymbol{\beta}^T = [\beta_0, \beta_1, \cdots, \beta_k, \beta_{11}, \cdots, \beta_{k,k}, \beta_{12}, \cdots, \beta_{k-1,k}]$$

and

$$\mathbf{X} = [\mathbf{1}, \mathbf{x}_1, \cdots, \mathbf{x}_k,\ \ \mathbf{x}_1^2, \cdots, \mathbf{x}_k^2,\ \ \mathbf{x}_1\mathbf{x}_2, \cdots, \mathbf{x}_{k-1}\mathbf{x}_k]$$

is the model matrix of order $n\times p$, structured for p parameters. $\mathbf{X}$ includes column of 1's and columns of linear, quadratic and interaction terms corresponding to $\boldsymbol{\beta}$.

2.1. Designs Under Study

We have chosen AP designs and subset designs for our study which are two relatively new classes of designs. AP designs were constructed for k=3, 4, 5, 6, 7, 8, 9, 10 in size n=15, 41, 41, 41, 41, 83, 83, 83 respectively with five center runs in each case. We have considered some cases by constructing subset designs of same size to compare with AP designs in the following examples and explored many other sizes in the Appendix B. The designs are also compared with CCD and BBD in the Appendices when all four types are available under a specific design size.

AP designs are a class of near saturated experimental designs, with three equally-spaced levels of each factor constructed for response surface modeling. The designs were constructed for the estimation of the second-order polynomial model by taking a k-factor initial factorial portion of n_1 runs from g columns of a Plackett-Burman (PB) plan, of Plackett and Burman (1946), with $k\leq g$. PB plans are economical screening designs based on Hadamard matrices and can estimate only a first order polynomial. The design size is a multiple of 4 starting from **an** 8-run design. PB design can be constructed by a cyclical rotation of an initial row or column of $+1$ **and** -1 and further adding a row or column of all $+1$s or -1s.

In the construction of AP design, the initial PB plan **of** n_1 **runs** was augmented by another set of $n_1(n_1-1)/2$ design points by taking the negative mean of each pair of (x_l, x_m) runs in the initial plan with $l<m$. The basic purpose was to provide better coverage of the experimental region than other standard designs. By the addition of **a** second portion to PB plan the designs become capable of estimating a second order model and **are** comparable to central composite designs (CCDs) of Box and Wilson (1951), Box-Behnken designs (BBDs) of Box and Behnken (1960) and small composite designs (SCDs) of Lin and Draper (1990) on the basis of run economy and generalized scaled prediction variances for the full model, for linear terms, for quadratic terms and for bilinear

terms. On some occasions, the AP design performed better than some other designs, especially SCDs. AP designs were also studied for different experimental regions; for example Fang and Mukerjee (2004) studied the optimal selection of AP designs, Tinsson (2007) investigated small size augmented pairs designs constructed for an initial saturated simplex design for two or three levels and Ahmad et al. (2012) discussed these designs for robustness to missing data both in cuboidal and spherical regions.

Table 1: General Structure of AP Design for k=5 with α_1=$\sqrt{k}$, α_2=$\sqrt{k/2}$ and α_3=$\sqrt{k/3}$ for an APS design and α_r=1 with r=1, 2, 3, for APC design.

center run replicates					S.No.	first-order plan(8 runs)					(x_l, x_m)	augmented runs($\binom{8}{2}$runs)				
0	0	0	0	0	1	1	1	1	-1	1	1,2	0	$-\alpha_2$	$-\alpha_2$	0	0
-	-	-	-	-	2	-1	1	1	1	-1	1,3	0	0	$-\alpha_2$	0	$-\alpha_2$
					3	-1	-1	1	1	1	1,4	$-\alpha_2$	0	0	0	$-\alpha_2$
					4	1	-1	-1	1	1	1,5	0	$-\alpha_3$	0	α_3	$-\alpha_3$
					5	-1	1	-1	-1	1	1,6	$-\alpha_3$	0	$-\alpha_3$	α_3	0
					6	1	-1	1	-1	-1	1,7	$-\alpha_2$	$-\alpha_2$	0	0	0
					7	1	1	-1	1	-1	1,8	0	0	0	α_1	0
					8	-1	-1	-1	-1	-1	2,3	α_3	0	$-\alpha_3$	$-\alpha_3$	0
											2,4	0	0	0	$-\alpha_1$	0
											2,5	α_2	$-\alpha_2$	0	0	0
											2,6	0	0	$-\alpha_2$	0	α_2
											2,7	0	$-\alpha_3$	0	$-\alpha_3$	α_3
											2,8	α_2	0	0	0	α_2
											3,4	0	α_3	0	$-\alpha_3$	$-\alpha_3$
											3,5	α_2	0	0	0	$-\alpha_2$
											3,6	0	α_2	$-\alpha_2$	0	0
											3,7	0	0	0	$-\alpha_1$	0
											3,8	α_2	α_2	0	0	0
											4,5	0	0	α_2	0	$-\alpha_2$
											4,6	$-\alpha_2$	α_2	0	0	0
											4,7	$-\alpha_3$	0	α_3	$-\alpha_3$	0
											4,8	0	α_2	α_2	0	0
											5,6	0	0	0	α_1	0
											5,7	0	$-\alpha_2$	α_2	0	0
											5,8	α_3	0	α_3	α_3	0
											6,7	$-\alpha_2$	0	0	0	α_2
											6,8	0	α_3	0	α_3	α_3
											7,8	0	0	α_2	0	α_2

Table 1 presents the general structure of an AP design for five factors. The first portion of the table represents center run replicates, the second portion contains five columns from 8-run Plackett-Burman plan and the third portion contains the augmented plan obtained by taking negative average of (x_l, x_m) pair of runs from the second portion. Throughout this paper, **an** AP design in a cuboidal region is represented as APC and **an** AP design in a spherical region is represented as APS. The number of factors are **indicated** as **a** subscript, for example, an AP design for k=3 in a spherical region is represented by APS_3.

A rich class of second-order response surface designs, called subset designs, which includes many popular second-order response surface designs like CCDs, BBDs, etc. **was proposed by Gilmour (2006)**. Subset designs are typically useful for experiments in which run-to-run variation is high, for example biological experiments. Designs are capable of estimating all second-order model terms, except quadratic terms, orthogonally. Subset designs are in general capable of running the experiment sequentially. The designs were constructed by using subsets from the regular 3^k factorial plans. If S_r, $r = 1, \ldots, k$, is the subset of runs of a 3^k factorial design lying on the hypersphere of radius $\sqrt{r}$ from the design center, S_0, then S_r contains all points with r factors at the ± 1 levels and the remaining $k - r$ factors at the 0 level. For a subset design in a spherical region of experimentation the axial **distances** α_r=$\sqrt{\frac{k}{r}}$, where r is number of non-zero factor levels in a run and α_r will be equal to 1 in a cuboidal region. A subset design is denoted as $c_0S_0 + c_1S_1 + \cdots + c_kS_k$, where the coefficient c_r is the number of replications of subset S_r. **The term** c_kS_k is the subset that contains all 2^k or 2^{k-p} factorial points. A subset design can estimate a second-order model, if $c_r > 0$ for at least two r and for at least one r with $1 \leq r \leq k$-1, to estimate all quadratic effects and c_r>0 for at least one r>1 to enable the estimation of all bilinear (interaction) effects. For a more detailed discussion of subset designs see Gilmour (2006) and Ahmad and Gilmour (2010).

As an example we have presented relevant subsets for k=4 in Table 2, in which $S_4/(1/2)S_4$ and $S_3/(1/2)S_3$ mention that the subset may contain all S_4 and S_3 type of points or respectively their half fractions. Whereas, α_1, α_2 and α_3 are non-zero levels of a factor **in the subsets** S_1**,** S_2 **and** S_3 **respectively,** their quantity will be 1 in a cuboidal region and $\sqrt{\frac{k}{r}}$ for r=$1, \ldots, k$, in a spherical region.

Table 2: Subsets for four factor subset designs

$S_4/(1/2)S_4$				$S_3/(1/2)S_3$				S_2				S_1			
-1	-1	-1	-1	$-\alpha_3$	$-\alpha_3$	$-\alpha_3$	0	$-\alpha_2$	$-\alpha_2$	0	0	$-\alpha_1$	0	0	0
$+1$	-1	-1	-1	$+\alpha_3$	$-\alpha_3$	$-\alpha_3$	0	$+\alpha_2$	$-\alpha_2$	0	0	$+\alpha_1$	0	0	0
-1	$+1$	-1	-1	$-\alpha_3$	$+\alpha_3$	$-\alpha_3$	0	$-\alpha_2$	$+\alpha_2$	0	0	0	$-\alpha_1$	0	0
$+1$	$+1$	-1	-1	$+\alpha_3$	$+\alpha_3$	$-\alpha_3$	0	$+\alpha_2$	$+\alpha_2$	0	0	0	$+\alpha_1$	0	0
-1	-1	$+1$	-1	$-\alpha_3$	$-\alpha_3$	$+\alpha_3$	0	$-\alpha_2$	0	$-\alpha_2$	0	0	0	$-\alpha_1$	0
$+1$	-1	$+1$	-1	$+\alpha_3$	$-\alpha_3$	$+\alpha_3$	0	$+\alpha_2$	0	$-\alpha_2$	0	0	0	$+\alpha_1$	0
-1	$+1$	$+1$	-1	$-\alpha_3$	$+\alpha_3$	$+\alpha_3$	0	$-\alpha_2$	0	$+\alpha_2$	0	0	0	0	$-\alpha_1$
$+1$	$+1$	$+1$	-1	$+\alpha_3$	$+\alpha_3$	$+\alpha_3$	0	$+\alpha_2$	0	$+\alpha_2$	0	0	0	0	$+\alpha_1$
-1	-1	-1	$+1$	$-\alpha_3$	$-\alpha_3$	0	$-\alpha_3$	0	$-\alpha_2$	$-\alpha_2$	0				
$+1$	-1	-1	$+1$	$+\alpha_3$	$-\alpha_3$	0	$-\alpha_3$	0	$+\alpha_2$	$-\alpha_2$	0				
-1	$+1$	-1	$+1$	$-\alpha_3$	$+\alpha_3$	0	$-\alpha_3$	0	$-\alpha_2$	$+\alpha_2$	0		S_0		
$+1$	$+1$	-1	$+1$	$+\alpha_3$	$+\alpha_3$	0	$-\alpha_3$	0	$+\alpha_2$	$+\alpha_2$	0	0	0	0	0
-1	-1	$+1$	$+1$	$-\alpha_3$	$-\alpha_3$	0	$+\alpha_3$	0	$-\alpha_2$	0	$-\alpha_2$				
$+1$	-1	$+1$	$+1$	$+\alpha_3$	$-\alpha_3$	0	$+\alpha_3$	0	$+\alpha_2$	0	$-\alpha_2$				
-1	$+1$	$+1$	$+1$	$-\alpha_3$	$+\alpha_3$	0	$+\alpha_3$	0	$-\alpha_2$	0	$+\alpha_2$				
$+1$	$+1$	$+1$	$+1$	$+\alpha_3$	$+\alpha_3$	0	$+\alpha_3$	0	$+\alpha_2$	0	$+\alpha_2$				
				$-\alpha_3$	0	$-\alpha_3$	$-\alpha_3$	$-\alpha_2$	0	0	$-\alpha_2$				
				$+\alpha_3$	0	$-\alpha_3$	$-\alpha_3$	$+\alpha_2$	0	0	$-\alpha_2$				
				$-\alpha_3$	0	$+\alpha_3$	$-\alpha_3$	$-\alpha_2$	0	0	$+\alpha_2$				
				$+\alpha_3$	0	$+\alpha_3$	$-\alpha_3$	$+\alpha_2$	0	0	$+\alpha_2$				
				$-\alpha_3$	0	$-\alpha_3$	$+\alpha_3$	0	0	$-\alpha_2$	$-\alpha_2$				
				$+\alpha_3$	0	$-\alpha_3$	$+\alpha_3$	0	0	$+\alpha_2$	$-\alpha_2$				
				$-\alpha_3$	0	$+\alpha_3$	$+\alpha_3$	0	0	$-\alpha_2$	$+\alpha_2$				
				$+\alpha_3$	0	$+\alpha_3$	$+\alpha_3$	0	0	$+\alpha_2$	$+\alpha_2$				
				0	$-\alpha_3$	$-\alpha_3$	$-\alpha_3$								
				0	$+\alpha_3$	$-\alpha_3$	$-\alpha_3$								
				0	$-\alpha_3$	$+\alpha_3$	$-\alpha_3$								
				0	$+\alpha_3$	$+\alpha_3$	$-\alpha_3$								
				0	$-\alpha_3$	$-\alpha_3$	$+\alpha_3$								
				0	$+\alpha_3$	$-\alpha_3$	$+\alpha_3$								
				0	$-\alpha_3$	$+\alpha_3$	$+\alpha_3$								
				0	$+\alpha_3$	$+\alpha_3$	$+\alpha_3$								

Some useful properties for fitting the second-order model under AP designs and subset designs are explored in Appendix A which presents the general structure of $\mathbf{X}^T\mathbf{X}$ for both designs. Both design classes, AP designs and subset designs, were originally presented as three level designs. We have theoretically computed the matrices of variances and covariances of regression coefficients for both classes in any region of experimentation in Appendix A.

3. Information Based Optimality Criteria

In this paper many optimality criteria are used to compare the two classes of response surface designs. These criteria are based on the information matrix $\mathbf{X}^T\mathbf{X}$ of the design under study, where $\mathbf{X}$ is the model matrix representing all terms of the second-order model. The information matrix of a design is used to compare designs as it is proportional to the inverse of the variance-covariance matrix of the design. The commonly used optimality criteria are D, A, E, G, I and I_D.

A design is called D-optimal if it maximizes the determinant of the information matrix. It may also be defined as,

$$D = min|\mathbf{X}^T\mathbf{X}|^{-1/p},$$

where p is the number of parameters in the model.

The A-optimality criterion minimizes the trace of the variance-covariance matrix of a design, i.e.

$$A = min\{trace(\mathbf{X}^T\mathbf{X})^{-1}\}.$$

E-optimality criterion minimizes the maximum eigenvalue (λ_{max}) of variance-covariance matrix, i.e.

$$E = min\{\lambda_{max}(\mathbf{X}^T\mathbf{X})^{-1}\}.$$

A prediction criterion is the G-optimality or global optimality criterion that minimizes the maximum prediction variance over the experimental space, as

$$G = min\{maxV(x, \xi)\}.$$

where the normalized generalization of $Var\{\hat{y}(\mathbf{x})\}$ when ξ is the probability measure on the experimental space of interest χ is $V(\mathbf{x}, \xi) = f^T(\mathbf{x})(\mathbf{X}^T\mathbf{X})^{-1}f(\mathbf{x})$, when $f(\mathbf{x})$ is the function of factor levels extended to the model terms.

I-optimality (integrated variance optimality) also called Q-optimality, V-optimality or I_v-optimality minimizes the average prediction variance of the estimated mean response,

$$I = min\frac{\int_{\chi} V(\mathbf{x}, \xi)dx}{\int_{x\in\chi} dx}.$$

The numerator of the above expression is simplified to $trace\{\mathbf{\Omega}(\mathbf{X}^T\mathbf{X})^{-1}\}$, where $\mathbf{\Omega} = \int_{x\in\chi} \mathbf{f^T}(\mathbf{x})\mathbf{f}(\mathbf{x})dx$

is the design moment in the region of interest. For more detailed description of alphabetic optimalities see Myers et al. (2009) and Atkinson et al. (2007).

In many situations the difference in response when factors are varied from one level to the other is more important than the actual value of the response. Trinca and Gilmour (2015) introduced the concept of integrated variance of the difference between the estimated response at a particular combination of factor levels $\mathbf{x}_a$ to the estimated response at the design center with factor levels $\mathbf{x}_0$. Hence the I_D-optimality criterion was defined as

$$I_D = min\frac{\int_{x\in\chi} Var(V(\mathbf{x},\xi) - V(\mathbf{x}_0,\xi))dx}{\int_{x\in\chi} dx}.$$

The above relation is proportional to,

$$min\frac{\int_{x\in\chi}\{(V(\mathbf{x_a}) - V(\mathbf{x_0})^T(\mathbf{X}^T\mathbf{X})^{-1}(V(\mathbf{x_a}) - V(\mathbf{x_0}))\}dx}{\int_{x\in\chi} dx} = min\frac{trace\{M_{x0}(\mathbf{X}^T\mathbf{X})^{-1}\}}{\int_{x\in\chi} dx},$$

where $M_{x0} = \int_{x\in\chi}\{(V(\mathbf{x}) - V(\mathbf{x_0})^T\}\{(V(\mathbf{x}) - V(\mathbf{x_0})\}dx$, $\mathbf{x}$ is the vector representing any combination of factor levels and $\mathbf{x_0}$ is the vector with all 0s, except the first entry, which is 1 in both vectors.

Though G-optimality ans I-optimality address prediction performance of a design but do not always truly explore the prediction ability of the competing designs. Giovannitti-Jensen and Myers (1989) presented variance dispersion graph (VDG) to examine the overall prediction capability of a design in spherical and cuboidal regions. VDG consists of line of maximum and minimum scaled prediction variances and their spherical averages over the spheres in experimental region. VDGs are quite useful but they do not provide full information about the distribution of scaled prediction variance. For this purpose, Zahran et al. (2003a) proposed fraction of design space (FDS) plot which provides complete structure of the prediction performance of a design. FDS plot gives volume of distribution of scaled prediction variance at different fractions of the design space.

We now compare AP designs and subset designs under the above mentioned optimality criteria for spherical and cuboidal regions. For a straightforward comparison of designs we compute efficiency of subset designs relative to the AP design in each case. Designs are also compared graphically in the fraction of design space plot for the estimated difference of response (DFDS) and the variance dispersion graph for estimated difference of response (DVDG). A DVDG shows the maximum and minimum prediction variance curves for each design, the maximum variance curve of each design being shown with double line width. Some useful subset designs for different sizes are presented in Appendix B.

4. Region of Experimentation

In experiments usually a region of experimentation or the ranges of included variables are predefined. The number of levels of each variable depends on the experimental region. Typically a cuboidal region or a spherical region of experiment is chosen. A cuboidal region may include points on vertices, center points, edge points and points on the face of a cube/hypercube. A spherical region allocates the design points on a sphere/hypersphere of radius usually $\sqrt{k}$ or at the center. A design can have different properties when employed in different regions. Location of a design point has an important role in the estimation of different model coefficients, for example the volume of a confidence ellipsoid changes with changes in the levels of variables.

4.1. Spherical Region

Some selected subset designs which are relatively more efficient are constructed on a sphere/hypersphere of $\sqrt{k}$ radius and compared with APS designs.

The comparison is presented in the following examples:

4.1.1. Example 1: k=3

Table 3 presents relative efficiencies of subset designs to AP design under different optimality criteria for three factors in a spherical region of experimentation. The APS_3 design is poor for all optimality criteria except for E-optimality where this design is better than S_3+S_1+S_0. The APS_3 design is especially very poor under G-optimality and A-optimality. Thus the AP design has very poor prediction capability as compared to subset designs. The AP design is also worse for integrated variance criteria, i.e. I-optimality and I_D-optimality. However, the APS_3 design does allow the maximum pure error degrees of freedom (PEDF).

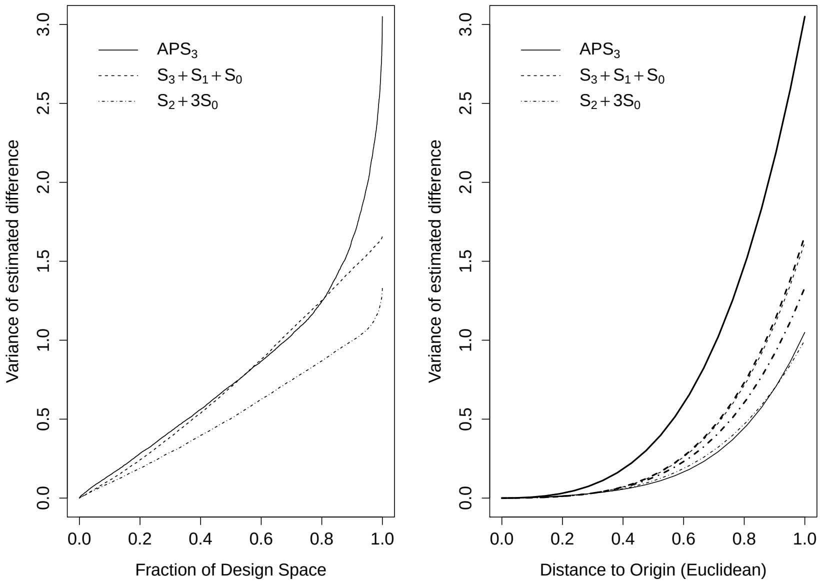

Figure 1: DFDS and DVDG of designs for k=3, n=15 in a spherical region

Table 3: Efficiency of subset designs relative to the AP design in a spherical region for k=3, n=15.

Design	PEDF	D-opt.	A-opt.	E-opt.	G-opt.	I-opt.	I_D-opt.
$S_3 + S_1$+S_0(CCD)	0	1.40	1.05	0.37	2.85	1.49	1.09
S_2+3S_0(BBD)	2	1.32	1.69	1.11	2.85	1.69	1.53
APS_3	4	1.00	1.00	1.00	1.00	1.00	1.00

Figure 1 shows DFDS plots and DVDGs of these designs in a spherical region. It can be observed from the DFDS that the APS_3 and S_3+S_1+S_0 designs are similar in 80% of the design space, but in the remaining space S_3+S_1+S_0 shows much lower prediction variances. The APS_3 design shows very high variance of estimated difference of response at the extremes of the design space. Clearly, the S_2+3S_0 design shows minimum variance of the estimated difference of response throughout the design space compared to the other two designs. In the DVDGs, we can observe from Figure 1 that APS_3 is very bad for maximum prediction variance, though this design is better for minimum prediction variance. The maximum and minimum prediction variance curves of S_3+S_1+S_0 almost coincide, indicating the near difference-rotatability property of the design. S_3+S_1+S_0 shows an overall better performance in the DVDG, showing the lowest curve for the maximum prediction variance and being very close **to** the lowest for the minimum prediction variance.

4.1.2. Example 2: k=4

Table 4 presents different relative efficiencies of designs for four factors in a spherical region. Some useful subset designs are compared with APS_4 design. APS_4 design is constructed by taking four columns from seven factor PB design which is a 2^{4-1}_{III} fraction as discussed in Ahmad et al. (2012). This fraction is augmented with 28 runs obtained by computing its pair-wise negative means. Adding five center runs, 41-run APS_4 design is obtained.

Table 4: Efficiency of subset designs relative to the AP design in a spherical region for k=4, n=41.

Design	PEDF	D-opt.	A-opt.	E-opt.	G-opt.	I-opt.	I_D-opt.
S_4+2S_1+9S_0	16	1.03	1.29	1.79	2.12	1.20	1.27
S_4+S_1+17S_0(CCD)	16	0.85	1.25	3.31	1.93	1.00	1.13
S_3+9S_0	8	0.96	1.29	1.79	1.13	1.00	1.08
S_2+S_1+9S_0	8	1.03	1.29	1.79	2.12	1.20	1.28
S_2+17S_0(BBD)	16	0.85	1.29	3.31	1.93	1.00	1.14
APS_4	10	1.00	1.00	1.00	1.00	1.00	1.00

In the case of D-optimality the subset design S_4+2S_1+9S_0 and S_2+S_1+9S_0 perform equally best, but the S_4+2S_1+9S_0 design allocates maximum degrees of freedom for estimating pure error.

The CCD and BBD perform identically under D-optimality but these designs are poorer than the APS_4 design. It is evident from Table 4 that all subset designs are better than APS_4 design under all other optimalities, in fact some are relatively much better.

Figure 2 displays DFDS plots and DVDGs for four factor 41-run designs in a spherical region. It can be observed from the DFDS plots that the APS_4 design shows higher variance for the estimated difference of response than the subset designs S_4+2S_1+9S_0 and S_2+S_1+9S_0 (both curves coincide), variance is particularly very high along the boundary of the sphere. In DVDGs for the estimated difference in response, we can see that the APS_4 design is very bad for the maximum difference of variances, whereas S_4+2S_1+9S_0 and S_2+S_1+9S_0 are equally much better than APS_4.

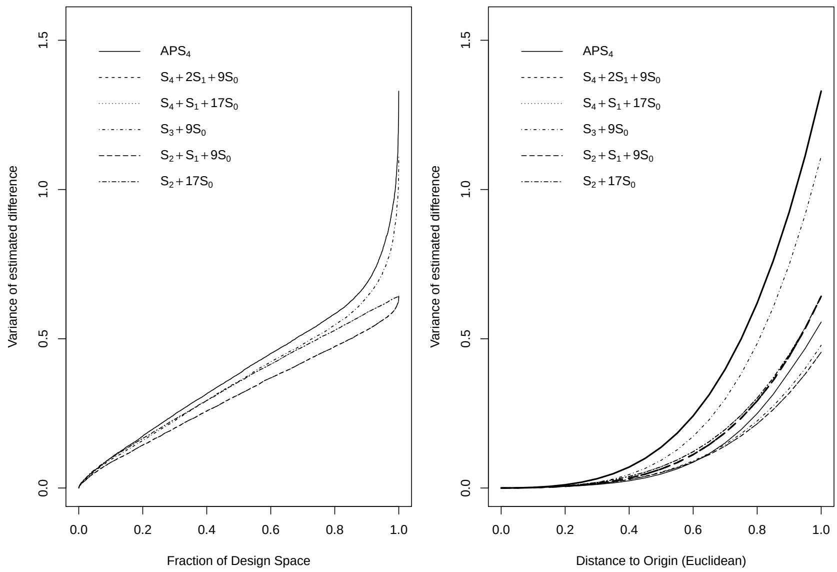

Figure 2: DFDS and DVDG for k=4, n=41 in a spherical region.

Table 5: Efficiency of subset designs relative to the AP design in a spherical region for k=5, n=41.

Design	PEDF	D-opt.	A-opt.	E-opt.	G-opt.	I-opt.	I_D-opt.
S_2+S_0(BBD)	0	1.08	0.53	0.20	0.86	1.01	0.57
(1/2)S_5+2S_1+5S_0	14	0.96	0.90	1.00	1.09	0.95	0.96
(1/2)S_4+S_0	0	0.83	0.45	0.20	0.49	0.63	0.45
APS_5	4	1.00	1.00	1.00	1.00	1.00	1.00

Similarly S_4+2S_1+9S_0 and S_2+S_1+9S_0 are also best for the minimum prediction variance than all other designs including APS_4. It is quite evident from both figures that S_4+2S_1+9S_0 and S_2+S_1+9S_0 are **the** best for predicting the difference of response in a spherical region.

4.1.3. Example 3: k=5

Four designs for five factors with 41 runs each are compared on the basis of different optimality criteria and their relative efficients are presented in Table 5. The results show that S_2+S_0 has the best performance under D- and I-optimality but this design is poor under other optimalities. This design also allots no degrees freedom to pure error. Subset design (1/2)S_5+2S_1+5S_0, in which a half fraction of resolution V was included, is quite close in performance to the APS_5 design but this design might be clearly preferred on the basis of degrees of freedom for pure error.

4.2. *Cuboidal Region*

Some selected subset designs are constructed for a cuboidal region of experimentation and compared with the APC design in the following examples.

4.2.1. *Example 4: k=3*

Relative efficiencies of some designs for three factors in a cuboidal region are presented in Table 6. Clearly, subset design S_3+S_1+S_0 shows the best performance under all optimality criteria but this design allots no degrees of freedom for pure error. The second best under these optimality criteria is S_2+3S_0 with two degrees of freedom for the estimation of pure error.

Table 6: Efficiency of subset designs relative to the AP design in a cuboidal region for k=3, n=15.

Design	PEDF	D-opt.	A-opt.	E-opt.	G-opt.	I-opt.	I_D-opt.
S_3+S_1+S_0(CCD)	0	1.97	2.36	2.28	8.76	2.52	3.02
S_2+3S_0(BBD)	2	1.61	2.22	1.86	5.06	2.41	2.36
APC_3	4	1.00	1.00	1.00	1.00	1.00	1.00

Figure 3 shows individual graphs of fractions of design space and variance dispersion graphs of the estimated difference of response. From the DFDS graphs we can see that subset designs are superior to the APC_3 design. From the DVDGs we can see that the APC_3 design is very bad for maximum prediction variance but this design is better than the S_2+3S_0 design for the minimum variance. Overall, performance of subset designs is better than APC_3 design.

4.2.2. *Example 5: k=4*

Table 7 presents relative efficiencies for four factor designs in a cuboidal region. The subset designs S_4+S_2+S_0, S_4+3S_1+S_0 and S_3+9S_0 are among the best designs under D-optimality but S_4+S_2+S_0 allots no degrees of freedom for pure error so this design might not be considered when pure error estimation is a priority. Under A-optimality best is S_3+9S_0 and some other subset designs, S_4+S_2+S_0, S_4+3S_1+S_0 and S_3+S_1+S_0, are also better than the APC_4 design. Under G-optimality, there are many subset deigns which are better than the APC_4 design.

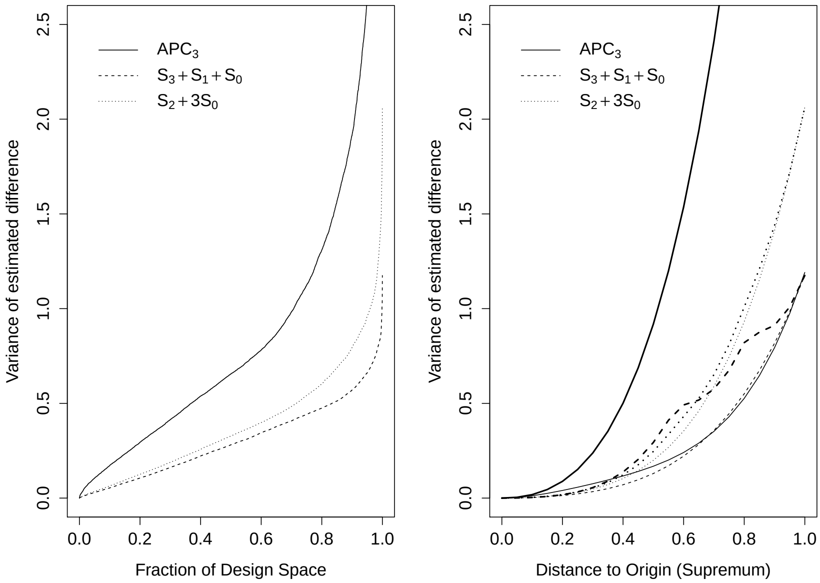

Figure 3: DFDS and DVDG for k=3, n=15 in a cuboidal region.

Table 7: Efficiency of subset designs relative to the AP design in a cuboidal region for k=4, n=41.

Design	PEDF	D-opt.	A-opt.	E-opt.	G-opt.	I-opt.	I_D-opt.
S_4+S_2+S_0	0	1.33	1.14	0.48	1.85	1.04	1.23
S_4+3S_1+S_0	16	1.12	1.06	0.77	1.48	1.08	1.16
S_3+S_1+S_0	0	1.21	1.06	0.38	1.52	0.98	1.06
S_3+9S_0	8	1.19	1.14	0.80	1.52	1.11	1.20
APC_4	10	1.00	1.00	1.00	1.00	1.00	1.00

From Table 7 it can be observed that whichever optimality criterion is chosen we can find some or many subset designs which are better than APC_4 design except under E-optimality where the APC_4 design is slightly better than subset designs S_4+3S_1+S_0 and S_3+9S_0. Under all optimality criteria, the overall performance of subset designs S_4+S_2+S_0, S_4+3S_1+S_0, S_3+S_1+S_0 and S_3+9S_0 is better in the cuboidal region.

DFDS plots and DVDGs for the variance of the estimated difference of response are presented in

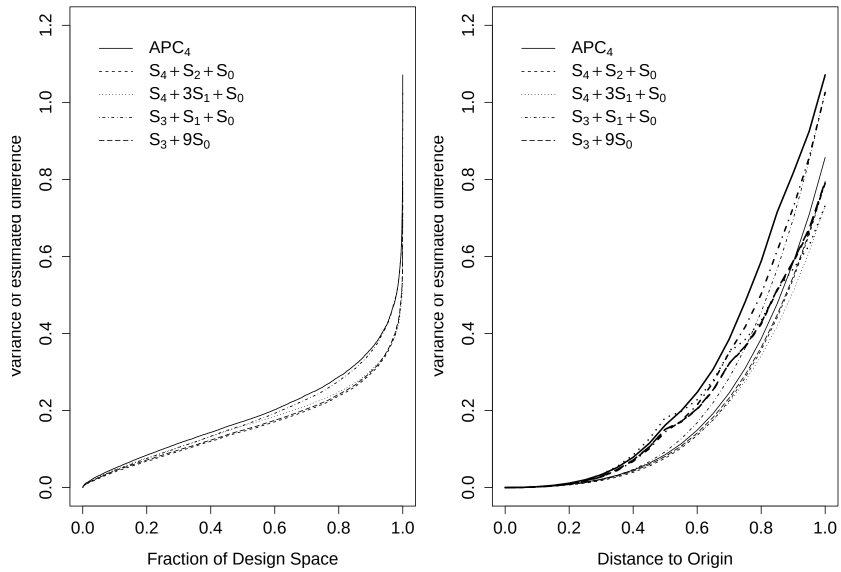

Figure 4: DFDS and DVDG for k=4, n=41 in a cuboidal region.

Figure 4. The subset designs S_4+S_2+S_0 and S_3+9S_0 show the lowest variation in the estimated difference of response throughout the design space, while the S_4+3S_1+S_0 design is the second best in the DFDS plot. The S_3+S_1+S_0 design also shows lower variance than APC_4 in almost 90% of the design space towards the center and in the remaining space this design shows equal variance to APC_4. In fact all the selected subset designs show overall better performance than the APC_4 design in DFDS plot. In the case of the DVDGs in Figure 4 we can see that the S_4+3S_1+S_0 and S_3+9S_0 designs are much better for maximum and minimum variance than APC_4 design. Curves of maximum and minimum prediction variance of both the designs coincide. The S_3+S_1+S_0 design also shows lower variation throughout the experimental region, while the S_4+3S_1+S_0 design gives slightly high variation in maximum variance in only 20% of the region. For minimum variance the APC_4 design is only better than the S_3+S_1+S_0 design in the region near the corners. It was observed in both the graphs that all curves of S_4+S_2+S_0 and S_3+9S_0 coincide. Thus we can find many subset design for four factors in 41 runs which can predict differences of response better than the APC_4 design in a cuboidal region.

4.2.3. *Example 6: k=5, cuboidal region*

A relative efficiency comparison of subset designs and the AP design for five factors in 41 runs in a cuboidal region is shown in Table 8. The overall performance of (1/2)S_5+2S_1+5S_0 is much

Table 8: Efficiency of subset designs relative to the AP design in a cuboidal region for k=5, n=41.

Design	PEDF	D-opt.	A-opt.	E-opt.	G-opt.	I-opt.	I_D-opt.
S_2+S_0(BBD)	0	0.58	0.40	0.11	0.44	0.39	0.25
(1/2)S_5+2S_1+5S_0	14	1.14	1.11	1.00	2.26	1.16	1.20
(1/2)S_4+S_0	0	1.42	0.82	0.19	1.55	0.36	0.82
APC_5	4	1.00	1.00	1.00	1.00	1.00	1.00

better than the other designs, though the APC_5 design has the same E-optimality and (1/2)S_4+S_0 is slightly better in terms of D-optimality.

5. Discussion

5.1. A catalogue of subset designs

We have shown that for up to five factors, subset designs outperform AP designs with the same number of runs. However, unlike AP designs, subset designs are not restricted to these specific run numbers. Indeed we can find good subset designs for many other cases. In Appendix B we show some of the most useful subset designs, along with their properties. The final choice of design will depend on the multiple objectives of the experiment and the advantages of simplicity in a particular application.

5.2. Final comments

In this paper, we have studied and compared subset designs and AP designs of the same size and many subset designs of other sizes for 3-6 factors, on the basis of different optimality criteria, both in a spherical region and in a cuboidal region of experimentation. Sometimes graphs can provide more detailed information as compared to numerical optimalities of a design. Thus designs are also studied using well known graphical comparison criteria like DFDS plot and DVDG drawn for differences of unscaled variances of predicted responses. We have shown that many subset designs outperform AP designs when compared under different alphabetic optimality criteria or graphically. It was observed that S_4+2S_1+9S_0 and S_2+S_1+9S_0 show all numeric and graphical properties similar to each other, except the number of degrees of freedom, in a spherical region of experimentation. Similarly, the pairs S_4+3S_1+S_0, S_2+2S_1+S_0 and S_4+S_1+17S_0, S_2+17S_0 also show identical numeric optimality measures, the only difference may be in the numbers of degrees of freedom. No such similarities among these designs were observed in a cuboidal region of experimentation. However, in the cuboidal region some designs behave identically in the prediction of differences of response, for example the curves of S_4+S_2+S_0 and S_3+9S_0 designs in DFDS plots and DVDGs coincide. We have considered many subset designs constructed with non-regular fraction which are sometime quite comparable to the designs constructed with regular fractions. For example (3/8)S_6+S_1+5S_0 performs better than other subset designs under A-, E- and I_D-optimality and **is** quite comparable to the APS_6 design under D-, A- and E-optimality as shown in Appendix B. Similarly (7/16)S_6+S_1+7S_0 design is comparable to other subset designs under different optimality criteria.

Using this paper, **the practitioners** will have a better choice of designs of the same size for small number of factors on the basis of their desirable optimality criterion and subset designs should be preferred to AP designs. On the other hand, the AP designs for larger number of factors can be quite useful when limited run size is the priority.

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Appendix A Variance-Covariance Structure of AP Designs and Subset Designs

The information matrix of both the classes of designs under study is of order p with the following general structure,

$$\mathbf{X}^T\mathbf{X} = \begin{pmatrix} \mathbf{\Delta} & \mathbf{0} \\ \mathbf{0} & \mathbf{\Gamma} \end{pmatrix},$$

where $\mathbf{\Delta}$ and $\mathbf{\Gamma}$ are square matrices of respective orders $\binom{k+1}{2}$ and $k+1$ and given as

$$\mathbf{\Delta}=\begin{pmatrix} \psi_1\mathbf{I}_k & \mathbf{C^T} \\ \mathbf{C} & \psi_2\mathbf{I}_k + \theta\mathbf{J}_k \end{pmatrix} \quad \text{and} \quad \mathbf{\Gamma}=\begin{pmatrix} n & \psi_1\mathbf{1^T} \\ \psi_1\mathbf{1} & \tau\mathbf{I}_k + \psi_2\mathbf{J}_k \end{pmatrix}.$$

The entries in $\mathbf{C}$ and θ are computed by $\sum_{j=1}^{n}\left(\prod_{i=1}^{k} x_{ij}\right)$, where x_{ij} represents the j^{th} level of the i^{th} factor. Some elements of $\mathbf{C}$ and θ are non-zero when a factorial fraction of resolution less than V is used in the subset design, or otherwise when some irregular fraction is used in an AP design, n is the number of design points. Note that $\mathbf{\Gamma}$ is of the same form as that given in the Appendix of Gilmour (2006).

For subset designs, ψ_1=$\sum_{r=1}^{k}\delta_r(\frac{r}{k})\alpha_r^2$, ψ_2=δ_k+$\sum_{r=2}^{k-1}\delta_r\{\frac{r(r-1)}{k(k-1)}\}\alpha_r^4$ and τ=$\sum_{r=1}^{k}\delta_r(\frac{r}{k})\alpha_r^4$. If δ_r represents the number of points of type S_r to be included in the subset design, then δ_r=$2^r\binom{k}{r}\nu_r$ for r=$0,1,\cdots,k$, where ν_r is the total number of replications of the rth subset with $\nu_r \geq 0 \ \forall \ r \in \{0,1,\cdots,k\}$. For example, for the design S_4+$\frac{1}{2}S_4$+S_1+$4S_0$, the value of ν_4=1+$\frac{1}{2}$, ψ_1=24+2α_1^2 and ψ_2=24.

For all AP designs constructed for $4 \leq k \leq 7$ by augmenting k columns from the 8-run Plackett-Burman design ψ_1=8+12α_r^2 and ψ_2=8+4α_r^4, whereas the AP designs for $8 \leq k \leq 11$ constructed by using columns from the 12-run Plackett-Burman plan have ψ_1=$12+30\alpha_r^2$ and ψ_2=$12+12\alpha_r^4$. The AP designs constructed for larger number of factors have similar patterns of ψ_1 and ψ_2 values.

In the above expressions, α_k is defined to be 1 and $\alpha_r \in \{1, \sqrt{k/r}\} \ \forall \ r$=$1,2,\cdots,k-1$.

Now

$$\mathbf{\Delta}^{-1} = \begin{pmatrix} \psi_1^{-1}(\mathbf{I}_k + \psi_1^{-1}\mathbf{C^T}\mathbf{S_B^{-1}}\mathbf{C}) & -\psi_1^{-1}\mathbf{C^T}\mathbf{S_B^{-1}} \\ -\psi_1^{-1}\mathbf{S_B^{-1}}\mathbf{C} & \mathbf{S_B^{-1}} \end{pmatrix}.$$

Let $\mathbf{B} = \psi_2\mathbf{I}_k + \theta\mathbf{J}_k$ then $\mathbf{S_B} = \mathbf{B} - \psi_1^{-1}\mathbf{C}\mathbf{C^T}$ is the Schur complement.

Since $|\mathbf{X}^T\mathbf{X}|$ is a block diagonal matrix, therefore $|\mathbf{X}^T\mathbf{X}| = |\mathbf{\Delta}|.|\mathbf{\Gamma}|$. We know that $|\Delta|$=$\psi_1^k|\mathbf{S_B}|$ and after some matrix algebra, we get

$$\begin{aligned} |\mathbf{\Gamma}| &= n.|(\tau - \psi_2)\mathbf{I}_k + \psi_2\mathbf{J}_k - \frac{\psi_1^2}{n}\mathbf{J}_k|, \\ &= (\tau - \psi_2)^{k-1}[-k\psi_1^2 + \{\tau + (k-1)\psi_2\}n]. \end{aligned}$$

The inverse of the information matrix is calculated directly by taking inverse of each matrix in the block diagonal matrix $\mathbf{X}^T\mathbf{X}$, where

$$\mathbf{\Gamma}^{-1} = \{\tau + (k-1)\psi_2\}\mathbf{I}_k + \frac{\{\tau + (k-1)\psi_2\}(\psi_1^2 - n\psi_2)}{k\psi_1^2 - \{\tau + (k-1)\psi_2\}n}\mathbf{J}_k - \frac{\psi_1^2(\tau - \psi_2)}{k\psi_1^2 - \{\tau + (k-1)\psi_2\}n}\mathbf{J}_k.$$

Then $\mathbf{\Gamma}^{-1}$ and $\mathbf{\Delta}^{-1}$ give the variances and covariances of the regression coefficient estimates of the assumed model. $\mathbf{\Gamma}^{-1}$ gives the variances of regression estimate of the constant term $var(\hat{\beta}_0)$, the k variances of the regression estimates of the quadratic terms i.e. $var(\hat{\beta}_{ii})$, and the covariances of the quadratic and constant terms i.e. $cov(\hat{\beta}_0, \hat{\beta}_{ii})\ \forall\ \ i$=$1, \cdots, k$. The remaining part of the matrix includes covariances of higher order terms. $\mathbf{\Delta}^{-1}$ computes variances of estimated linear and bilinear regression coefficients on the diagonal and variances of higher order coefficients at off-diagonal locations. An important reference for the details of above used matrix algebra is Searle (2000).